Gaussian quantum fluctuations in interacting many particle systems

A Lyapunov type central limit theorem for mixing quantum systems

Michael Hartmann (`michael.hartmann@dlr.de`)
Institute of Thechnical Physics, DLR Stuttgart and
Institute of Theoretical Physics I, University of Stuttgart

Günter Mahler
Institute of Theoretical Physics I, University of Stuttgart

Ortwin Hess
Advanced Technology Institute, University of Surrey

February 7, 2008

Abstract. We consider a many particle quantum system, in which each particle interacts only with its nearest neighbours. Provided that the energy per particle has an upper bound, we show, that the energy distribution of almost every product state becomes a Gaussian normal distribution in the limit of infinite number of particles. We indicate some possible applications.

Physical systems, composed of interacting identical (or similar) subsystems appear in many branches of physics. They are standard in condensed matter physics.

Assuming that each subsystem only interacts with its nearest neighbours and that the energy per subsystem has an upper limit, which must not depend on the number of subsystems n, we show that the distribution of energy eigenvalues of almost every product state converges to the Gaussian normal distribution in the limit of infinitely many subsystems. To the best of our knowledge, this fundamental quantum feature has not yet been recognized in the literature [1, 2, 3].

Central limit theorems for the distribution of energy eigenvalues in quantum gases with Boltzmann statistics [4] as well as for Bose and Fermi statistics [5] have been discussed by M. Sh. Goldstein. His theorems apply for mixed states, namely classical mixtures of quantum states involving classical probabilities.

We consider here the distribution of energy eigenvalues for a pure quantum state. In our case, the distribution is thus of purely quantum nature, it solely exists because the state we consider is not an eigenstate of the energy operator of our system. Our theorem may be viewed as a central limit theorem for mixing quantum systems.

Some extensions of the central limit theorem to quantum systems, with the state not necessarily being mixed, have been proven in the past [6, 7, 8, 9, 10, 11]. The version, which appears closest related to ours, has been published by Goderis and Vets in 1989 [9]. They consider a quantum lattice system and assume that the state and the operator, they look at, are invariant under lattice translations. Their proof is then based on a set of "cluster conditions", which replace the mixing condition of the random variable case.

The assumptions we use are stricter with respect to the mixing behavior, nevertheless, they may still be weakened and generalised. On the other hand, we do not assume translational invariance of the operators or the state. Instead, we use a quantum analogue of the Lyapunov condition for random variables. This generalisation opens up a large field of applications. The version of Coderis and Vets only applies to products of identical subsystem states, while ours applies to almost every product state with the fraction of exceptions being negligible.

Knowing the energy distribution of a product state one can deduce estimates on various quantities of interest. If the system is known to be in a product state at some initial time, one can calculate it's energy distribution. As this distribution is conserved under Schrödinger dynamics, one can then make predictions on the dynamics of the state, even in the long time limit. These circumstances should prove helpful in many problems related to chaotic or non-chaotic behavior in quantum systems.

On the other hand, for a given global state of the total system being a function of the total Hamiltonian H, one can calculate occupation probabilities of product states. Since only in the product basis traces over single subsystems can be performed, this procedure allows to calculate properties of the reduced density matrix of any subsystem. In this way, one could analyse the local properies of stationary global states.

Finally, our theorem may underly the often-used assumption of Gaussian fluctuations.

Notation: We first give some notation and definitions we use: We consider a chain of quantum systems with next neighbour interactions. Let the entire system be described by a Hamiltonian H which is a linear, self-adjoint operator on a seperable, complex Hilbert space $\mathscr{H}$. The Hilbert space $\mathscr{H}$ is a direct product of the Hilbert spaces of the subsystems,

$$\mathscr{H} \equiv \prod_{\mu=1}^{n} \otimes \mathscr{H}_{\mu}, \tag{1}$$

and the Hamiltonian may be written in the form,

$$H \equiv \sum_{\mu=1}^{n} \mathcal{H}_{\mu}, \qquad (2)$$

with

$$\mathcal{H}_{\mu} \equiv \mathbf{I}^{\otimes \mu-1} \otimes H_{\mu} \otimes \mathbf{I}^{\otimes n-\mu} + \mathbf{I}^{\otimes \mu-1} \otimes I_{\mu,\mu+1} \otimes \mathbf{I}^{\otimes n-(\mu+1)}, \qquad (3)$$

where H_{μ} is the proper Hamiltonian of subsystem μ, and $I_{\mu,\mu+1}$ the interaction of subsystem μ with subsystem $\mu + 1$. $\mathbf{I}$ is the identity operator. We chose the boundary condition $I_{n,n+1} = 0$.

Let E_{φ} be the eigenenergies and, using the Dirac notation [12], let $\{|\varphi\rangle\}$ be an orthonormal basis of $\mathscr{H}$ consisting of eigenstates of the total system.

$$H|\varphi\rangle = E_{\varphi}|\varphi\rangle \quad \text{with} \quad \langle\varphi|\varphi'\rangle = \delta_{\varphi\varphi'}, \qquad (4)$$

where $\delta_{\varphi\varphi'}$ is the Kronecker delta. We denote by $|a\rangle$ the product state

$$|a\rangle \equiv \prod_{\mu=1}^{n} \otimes |a_{\mu}\rangle, \qquad (5)$$

built up from some state $|a_{\mu}\rangle$ of each subsystem μ, $|a_{\mu}\rangle \in \mathscr{H}_{\mu}$.

We furthermore define,

$$\overline{E}_a \equiv \langle a|H|a\rangle \qquad (6)$$
$$\sigma_a^2 \equiv \langle a|H^2|a\rangle - \langle a|H|a\rangle^2, \qquad (7)$$

and introduce the operator

$$Z_n \equiv \frac{H - \overline{E}_a}{\sigma_a} \qquad (8)$$

which is diagonal in the same basis as H. Let z_{φ} denote its eigenvalues,

$$Z_n|\varphi\rangle = z_{\varphi}|\varphi\rangle. \qquad (9)$$

Note that H and therefore $\overline{E}_a$, σ_a and z_{φ} as well as the basis $\{|\varphi\rangle\}$ depend on n.

Since H and thus Z_n are self-adjoint, $|a\rangle$ induces a measure on the spectrum of Z_n respective H. This measure of the quantum mechanical distribution of the eigenvalues of Z_n in the state $|a\rangle$, is given by the usual formula,

$$\mathbb{P}_a\left(z_{\varphi} \in [z_1, z_2]\right) = \sum_{\{|\varphi\rangle : z_1 \leq z_{\varphi} \leq z_2\}} |\langle a|\varphi\rangle|^2, \qquad (10)$$

4

where the sum extends over all states $|\varphi\rangle$ with eigenvalues in the respective interval.

Theorem: If the operator H and the state $|a\rangle$ satisfy

$$\sigma_a^2 \geq n\,C \tag{11}$$

for all n and some $C > 0$ and if each operator $\mathcal{H}_\mu$ is bounded, i.e.

$$\langle \chi | \mathcal{H}_\mu | \chi \rangle \leq C' \tag{12}$$

for all normalised states $|\chi\rangle \in \mathscr{H}$ and some constant C', then the quantum mechanical distribution of the eigenvalues of Z_n in the state $|a\rangle$ converges weakly to a Gaussian normal distribution:

$$\lim_{n \to \infty} \mathbb{P}_a\left(z_\varphi \in [z_1, z_2] \right) = \int_{z_1}^{z_2} \frac{\exp\left(-z^2/2 \right)}{\sqrt{2\pi}}\, dz \tag{13}$$

for all $-\infty < z_1 < z_2 < \infty$.

Proof: Following the proof of the central limit theorem for mixing sequences [13] as a guideline, we prove the statement (13) in three steps: First, we show that the characteristic function of H does not change if a few of the $\mathcal{H}_\mu$ are neglected. Second, we prove, that the characteristic function of the remainder of H factorises. In the last step, we then show that the condition for Lyapunov's version of the central limit theorem is fulfilled for the remainder of H. The proof is then completed by the standard proof of Lyapunov's central limit theorem, which can be found in several textbooks [14].

Define the operators $X_\mu \equiv \mathcal{H}_\mu - \langle a | \mathcal{H}_\mu | a \rangle$ and split the sum

$$Z_n = \frac{1}{\sigma_a} \sum_{\mu=1}^{n} X_\mu \tag{14}$$

into alternate blocks of length $k-1$ (large blocks) and of length 1 (small blocks). The large blocks are given by

$$\xi_j = \sum_{l=1}^{k-1} X_{(j-1)\cdot k + l} \quad \text{for} \quad j = 1, \ldots, [n/k] \quad \text{and} \tag{15}$$

$$\xi_{[n/k]+1} = \sum_{l=1}^{q} X_{[n/k]\cdot k + l} \quad \text{with} \quad q = n - k\,[n/k], \tag{16}$$

where $[x]$ means the integer part of x and the small blocks are the $X_{j \cdot k}$ with $j = 1, \ldots, [n/k]$. Sum up all large blocks and all small blocks separately,

$$Z_n' = \frac{1}{\sigma_a} \sum_{j=1}^{[n/k]+1} \xi_j \quad \text{and} \quad Z_n'' = \frac{1}{\sigma_a} \sum_{j=1}^{[n/k]} X_{j \cdot k}, \tag{17}$$

so that $Z_n = Z'_n + Z''_n$. The integer block length k is chosen to depend on n $(k = k(n))$ such that

$$\lim_{n \to \infty} \frac{n}{k^2} = 0 \quad \text{and} \quad \lim_{n \to \infty} \frac{k}{n} = 0, \tag{18}$$

with $k = \left\lceil n^{3/4} \right\rceil$ being a possible realisation.

Consider the characteristic function

$$\langle a | e^{-ir Z_n} | a \rangle \tag{19}$$

with real r.

First let us show that for all real r and $n \to \infty$:

$$\langle a | e^{-ir Z_n} | a \rangle \to \langle a | e^{-ir Z'_n} | a \rangle \tag{20}$$

Using the operator identity [15]

$$e^{-ir(A+B)} = e^{-irA} - i \int_0^r e^{-i(r-s)(A+B)} B e^{-isA} ds, \tag{21}$$

the triangle- and the Schwarz-inequality, one gets

$$\left| \langle a | e^{-ir Z_n} - e^{-ir Z'_n} | a \rangle \right| \leq \int_0^r ds \sqrt{\langle a | e^{is Z_n} \left(Z''_n \right)^2 e^{-is Z_n} | a \rangle}$$

$$\leq r \sqrt{\left(\frac{1}{n} \left[\frac{n}{k} \right]^2 \right) \frac{(2C')^2}{C}} \tag{22}$$

which, indeed, converges to zero for $n \to \infty$.

Next, we show that the characteristic function of Z'_n factorises.

$$\langle a | e^{-ir Z'_n} | a \rangle = \prod_{j=1}^{[n/k]+1} \langle a | e^{-ir \xi_j} | a \rangle \tag{23}$$

To this end, we first note two important properties that arise due to the next neighbour interaction and the product property of the state $|a\rangle$: For $|\mu - \nu| > 1$ and any two integers k and l, we have

$$[\mathcal{H}_\mu, \mathcal{H}_\nu] = 0 \tag{24}$$

$$\langle a | \left(\mathcal{H}_\mu \right)^k \left(\mathcal{H}_\nu \right)^l | a \rangle = \langle a | \left(\mathcal{H}_\mu \right)^k | a \rangle \langle a | \left(\mathcal{H}_\nu \right)^l | a \rangle. \tag{25}$$

Therefore, for all (i, j) and any two integers k and l,

$$[\xi_i, \xi_j] = 0 \tag{26}$$

$$\langle a | \left(\xi_i \right)^k \left(\xi_j \right)^l | a \rangle = \langle a | \left(\xi_i \right)^k | a \rangle \langle a | \left(\xi_j \right)^l | a \rangle, \tag{27}$$

and equation (23) follows as a direct consequence.

Finally we prove that the ξ_j fulfill the Lyapunov condition:

$$\lim_{n\to\infty} \frac{1}{\sigma_a^{2+m}} \sum_{j=1}^{[n/k]+1} \langle a| \, |\xi_j|^{2+m} \, |a\rangle = 0 \qquad (28)$$

for some $m > 0$. Note that due to equation (20), $\langle a| \, (Z_n')^2 \, |a\rangle \to \sigma_a^2$ as $n \to \infty$ and therefore equation (28) is, indeed, the Lyapunov condition for the ξ_j. We verify the condition for $m = 2$. To this end, consider

$$\langle a|\xi_j^4|a\rangle = \sum_{\mu,\nu,\rho,\tau=1}^{k-1} \langle a|X_{(j-1)k+\mu} X_{(j-1)k+\nu} X_{(j-1)k+\rho} X_{(j-1)k+\tau}|a\rangle. \qquad (29)$$

Since $\langle a|X_\mu|a\rangle = 0$ and because of equations (26) and (27), only those terms are nonzero, for which all the X_μ are identical or neighbours or where two pairs of identical or neighbouring X_μ appear. For example $\langle a|X_\mu X_{\mu+1} X_{\mu+2} X_{\mu-1}|a\rangle \neq 0$ while $\langle a|X_\mu X_{\mu+1} X_{\mu+3} X_{\mu-1}|a\rangle = 0$ or $\langle a|X_\mu X_{\mu+1} X_{\nu-1} X_\nu|a\rangle \neq 0$ while $\langle a|X_\mu X_\nu X_\mu X_{\nu+2}|a\rangle = 0$. Using this fact and the conditions (11) and (12) one realises that

$$\frac{1}{\sigma_a^4} \sum_{j=1}^{[n/k]+1} \langle a|\xi_j^4|a\rangle \leq$$

$$\leq \left(\left[\frac{n}{k}\right] + 1\right) \frac{((k-1)^2 + 3\cdot 5\cdot 7\cdot 3! \cdot (k-1))\,(2C')^4}{n^2 C^2} \qquad (30)$$

where the rhs vanishes in the limit $n \to \infty$. Note that $\langle a|\xi_{[n/k]+1}^4|a\rangle$ contains less terms than $\langle a|\xi_j^4|a\rangle$ for $j < [n/k]+1$ and is therefore bounded by the same expression.

With the arguments above showing that the characteristic function of Z_n' factorises and that the ξ_j obey the Lyapunov condition, it is straight forward to prove, following the standard steps [14], that

$$\lim_{n\to\infty} \langle a| \exp\left(-i\,r\,Z_n'\right) |a\rangle = \exp\left(-\frac{r^2}{2}\right) \qquad (31)$$

and, using equation (20) one concludes that

$$\lim_{n\to\infty} \langle a| \exp\left(-i\,r\,Z_n\right) |a\rangle = \exp\left(-\frac{r^2}{2}\right). \qquad (32)$$

Here both limits are pointwise for all real r.

Finally, the continuity theorem [14] states that the pointwise convergence of the characteristic functions, established above, implies the

weak convergence of the distributions. The density of the limit distribution is thus given by the Fourier transform of the characteristic function in equation (32), which proves our theorem.

Note that all the steps not explicitly carried out here only use properties of Lebesgue integration and no further properties of probability distributions. We therefore do not run into difficulties related to so called "no hidden variable theorems" [16, 17].

For applications in physics, where n is very large but finite, the density of the limit distribution can be written as a function of the energy E of the system,

$$\rho_a(E) = \frac{1}{\sqrt{2\pi}\,\sigma_a}\,\exp\left(-\frac{\left(E - \overline{E}_a\right)^2}{2\,\sigma_a^2}\right),\qquad(33)$$

so that $\mathbb{P}_a(E \in [E_1, E_2]) = \int_{E_1}^{E_2} \rho_a(E)dE$.

Discussion and Generalisations: Let us first analyse the conditions (11) and (12) in more detail.

Rewriting (11) in terms of the operators X_μ and using equation (25) we get

$$\sum_{\mu=1}^{n}\langle a|\frac{1}{2}\left(X_\mu^2 + X_{\mu+1}^2\right) + X_\mu X_{\mu+1} + X_{\mu+1}X_\mu|a\rangle \geq nC.\qquad(34)$$

Thus, every term in the sum in (34) being larger than C is sufficient for (11) to be satisfied.

Condition (12) physically states, that the excitation energy must not be concentrated in only a small part of the subsystems. For very large systems, where our theorem applies, this is only a minor restriction since the fraction of states that do not fulfill condition (12) is vanishingly small.

Several conditions we have used to derive our theorem may be relaxed and substituted by weaker assumptions.

First of all, the theorem is not only valid for a linear chain but also for two and three dimensional lattices.

It is also straight forward to proof the same theorem for periodic boundary conditions, $I_{n,n+1} = I_{n,1}$.

In addition, it is obviously not necessary that the subsystems only interact with their nearest neighbours. The theorem holds as long as the number of interaction partners (the connectivity) of each particle is limited.

Furthermore, the observable one considers need not be the Hamiltonian. Any other observable shows the same feature as long as conditions (11), (12), (24) and (25) are met.

Let us stress here, that neither the operator (Hamiltonian) nor the product state need to be invariant with respect to lattice translations.

Finally, conditions (11) and (12) may be relaxed, since the theorem still holds, whenever Lyapunov's condition, or even only Lindeberg's condition [14], is fulfilled. We have chosen here stricter but simpler conditions to make it easier to check the applicability of our theorem.

Examples: We mention two examples, where our theorem applies. First, we consider an Ising spin chain of the type [18]

$$H = -B \sum_i s_i^z - \frac{J}{2} \sum_i s_i^x \otimes s_{i+1}^x. \qquad (35)$$

Here, s_i^x and s_i^z are the Pauli matrices,

$$s^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad s^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad (36)$$

B the difference between local energy levels and J the coupling strength. The energy of each spin is at least $-B$ and at most B so that condition (12) is satisfied. The squared width σ_a^2 reads

$$\sigma_a^2 = n \frac{J^2}{4}, \qquad (37)$$

where n is the number of spins, and condition (11) is also met.

As a second example, we consider a harmonic chain.

$$H = -\sum_i \frac{p_i^2}{2m} + \frac{m}{2} \omega^2 \left(q_{i+1} - q_i \right)^2 \qquad (38)$$

where q_i and p_i are the position and momentum of particle number i. All particles have mass m and the coupling has frequency ω. Since the energy of a harmonic oscillator is not bounded, our theorem only applies to states where the energy per oscillator does not exceed a certain bound, which on the other hand may be chosen arbitrarily large. The squared width σ_a^2 for the harmonic chain is

$$\sigma_a^2 = n \omega^2 \left(n_i + \frac{1}{2} \right) \left(n_{i+1} + \frac{1}{2} \right) \qquad (39)$$

where n_i is the occupation number of oscillator number i. Since $n_i \geq 0$, condition (11) is satisfied.

Applications: We finally discuss two areas of possible applications of our result.

a: One may consider the product state $|a\rangle$ as an initial state and make predictions about its dynamics. Using equation (32), one can

calculate the fidelity of state $|a\rangle$:

$$\left|\langle a|e^{-iHt}|a\rangle\right|^2 = e^{-\sigma_a^2 t^2} \tag{40}$$

Furthermore, one can give an upper bound to the transition probability to another product state $|b\rangle$ ($\langle a|b\rangle = 0$) for all times t;

$$\left|\langle b|e^{-iHt}|a\rangle\right|^2 \leq \frac{2\,\sigma_a\,\sigma_b}{\sigma_a^2 + \sigma_b^2}\ \exp\left(-\frac{\left(\overline{E}_a - \overline{E}_b\right)^2}{2(\sigma_a^2 + \sigma_b^2)}\right) \tag{41}$$

where we have assumed $\sigma_a \ll \overline{E}_a$ and $\sigma_b \ll \overline{E}_b$ and the ground state energy has been chosen to be zero ($E_0 = 0$).

b: One can calculate diagonal elements of the reduced density matrix of a selected subsystem in the basis $|a_\mu\rangle$, provided the total system is in a stationary state, that is, its density matrix ρ_{total} is a function of H [19]. For this applications, it is most interesting to take $|a\rangle$ to be an eigenstate of the Hamilton operator without the nearest neighbour interactions ($H_0|a\rangle = E_a|a\rangle$, $H_0 = \sum_\mu H_\mu$). Here, very interesting conclusions can be drawn on the minimal spatial extension of temperature, which will be presented elsewhere [20].

In summary, we have considered a large quantum system composed of subsystems, where each subsytem only interacts with a limited number of neighbours. We have shown that for almost every product state, the distribution of the total energy converges to a Gaussian normal distribution in the limit of infinitely many subsystems (13). This is the main result of this paper. The assumptions we have made are quantum mechanical analogues to the conditions for Lyapunov's central limit theorem for mixing random variables. We did not dwell on the most general assumptions needed for our theorem to make the verification of our conditions in physical applications straightforward. Nevertheless we have discussed possible generalisations as well as some preliminary applications.

References

1. Lieb, E. and Mattis, D.: 1966, 'Mathematical Physics in One Dimension', Academic Press, New York
2. Thirring W.: 2002, 'Quantum Mathematical Physics' Springer , Berlin, 2nd ed.

3. Lieb, E.: 2001, 'The Stability of Matter: From Atoms to Stars', Springer , Berlin
4. Goldstein M. Sh.: 1985 *J. Stat. Phys.* **40**, pp. 329
5. Goldstein M. Sh.: 1985 *Theoret. and Math. Phys.* **1**, pp. 412
6. Cushen, C.D. and Hudson, R.L.: 1971 *J. Appl. Probability* **8**, pp. 454
7. Accardi, L. and Bach, A.: 1985, *Z. Wahrsch. verw. Geb.* **68**, pp. 393
8. Goderis, D., Verbeure, A. and Vets, P.: 1989, *Prob. Th. Rel. Fields* **82**, pp. 527
9. Goderis, D. and Vets, P.: 1989, *Comm. Math. Phys.* **122**, pp. 249
10. Kuperberg G.: 2002, *math-ph/0202035*
11. Michoel, T. and Nachtergaele, B.: 2003, *math-ph/0310027.*
12. Sakurai, J.J.: 1994, 'Modern Quantum Mechanics', Addison-Wesley, Reading, Massachusetts
13. Ibargimov, I.A. and Linnik, Y.V.: 1971, 'Independent and Stationary Sequences of Random Variables', Wolters-Noordhoff, Groningen/Netherlands
14. Billingsley, P.: 1995, 'Probability and Measure', John Wiley & Sons, New York, 3rd ed.
15. Fick, E. and Sauermann, G.: 1990, 'The Quantum Statistics of Dynamic Processes', Springer , Berlin
16. Dürr, D., Goldstein, S., Zanghi, N.: 2003, *J. Stat. Phys.* **67** pp. 843
17. Dürr, D., Goldstein, S., Zanghi, N.: 2004, *J. Stat. Phys.* to be published, *quant-ph/0308038*
18. Mahler, G. and Weberruß, V.: 2001, 'Quantum Networks', Springer , Berlin
19. Jordan, A.N. and Büttiker, M.: 2003, *cond-mat/0311647*
20. Hartmann, M., Mahler, G. and Hess, O.: *quant-ph/0312214*